A New Approximation of the Equation of State for Sea Water, Suitable for Numerical Ocean Models

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Abstract

An approximation to the UNESCO equation of state for sea water is obtained in the form of a polynomial that is cubic in potential temperature, quadratic in pressure, and linear in salinity. The polynomial represents a reasonable compromise between accuracy and computational economy; it also allows potential temperature to be obtained analytically from given values of density, salinity and pressure.

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1 Introduction

The equation of state for sea water, which links density (ρ) to temperature (T), salinity (S), and pressure (p), is a rather complex mathematical expression. For example, the formula of Millero et al. (1980), usually referred to as the UNESCO formula, involves a 26-term polynomial of 4th degree in T, 2nd degree in p, and of 1.5^{th} degree in S. The high computational burden placed by this equation on numerical ocean circulation models has spawned attempts to approximate the "exact" equation by simpler formulae. The present paper represents one such attempt.

In isopycnic ocean modeling and data analysis, the need frequently arises to diagnose temperature (or salinity) for given values of density, pressure, and salinity (or temperature, as the case may be). In principle, this can be done by solving the UNESCO formula iteratively. Experience shows, however, that systematic errors inherent in iterative methods, no matter how small, will accumulate over time if the numerical algorithm in an ocean model calls for evaluation of both $\rho(T, S, p)$ and $T(\rho, S, p)$ at each model time step, that is, if the equation of state is solved back and forth many times.

Bryan and Cox (1972) simplified the density calculation by expressing density *anomalies* at fixed depth levels by a 3rd degree polynomial in T and S. Friedrich and Levitus (1972, hereafter FL) fitted a polynomial cubic in T, quadratic in depth, and linear in S to the Knudsen-Ekman formula (Forsch *et al.*, 1902; Ekman, 1908). The FL formula simplifies the equation of state to the point where $T(\rho, S, p)$ and/or $S(\rho, T, p)$ can be obtained analytically, thus avoiding the accumulation of numerical biases in back-and-forth applications like those necessary in isopycnic models. Levitus and Isayev (1992, hereafter LI) updated FL (1972) by fitting the same polynomial to the UNESCO equation of state.

Both the Knudsen-Ekman and the UNESCO formula use *in situ* temperature as one of the variables, while in many oceanographic applications potential temperature (θ) is used due to its entropy-conserving properties. The error introduced by not distinguishing between T and θ in the equation of state are not negligible, as pointed out by Mellor (1991). He estimated this difference and gave a correction formula. More recently, Jackett and McDougall (1995,

hereafter JMcD) modified the UNESCO formula so that it is written directly in terms of θ instead of T.

In this paper, we combine the approaches taken by JMcD and LI. Specifically, we generate a polynomial in θ, S, and p representing a best fit to the UNESCO equation of state. This polynomial is intended for use in ocean models where computational expense is an issue, where θ replaces T as the variable describing the temperature field, and where the equation of state must be invertible, i.e., must be solvable for θ as a function of ρ, S, p.

2   Two-stage procedure used to fit the JMcD formula

The JMcD formula is of the form

$$\rho(\theta, S, p) = \frac{\rho(\theta, S, 0)}{1 - p/K(\theta, S, p)}, \tag{1}$$

where $\rho(\theta, S, 0) = \rho(T, S, 0)$ (since $\theta = T$ at $p = 0$) is a 15-term equation in powers of S and T, and $K(\theta, S, p)$ is a 26-term equation in powers of θ, S, and p.

Following FL and LI, we approximate (1) by a seven-term polynomial cubic in θ and linear in S:

$$\sigma(\theta, S, p) = C_1(p) + C_2(p)\theta + C_3(p)S + C_4(p)\theta^2 + C_5(p)S\theta + C_6(p)\theta^3 + C_7(p)S\theta^2, \tag{2}$$

where $\sigma = \rho$ - $1000 \, \mathrm{kg \, m^{-3}}$.

The potential temperature, salinity and pressure ranges used in this fit are shown in Table 1. Note that we fit a single polynomial (2) over a depth-independent range of θ and S to assure accurate calculation of surface water potential density referenced to greater depths. (Again, this is a special concern in isopycnic modeling.) In contrast, both FL and LI narrowed the temperature and salinity range considerably at depths, and FL reduced the number of terms in (2) from seven to five there. Using different polynomials at different depths is safe in models whose coordinate surfaces are at fixed depth levels but is inappropriate in models where pressure on individual coordinate surfaces varies continually in space and time.

The coefficients $C_{1...7}$ were determined in a manner closely following FL and LI: In the first stage, a least-squares fit of $\sigma(\theta, S, p)$ in (2) to the JMcD formula (1) was carried out over the prescribed range of θ and S shown in Table 1 for discrete values of p ranging from 0 to 50 MPa in increments of 1 MPa (approximately 0 to 5000 m in increments of 100 m). This yielded 50 values for each C_N, corresponding to 50 discrete pressure levels. In the second stage, a quadratic polynomial in p was fitted to each of these sets of 50 values, resulting in expressions

$$C_N(p) = \alpha_N + \beta_N p + \gamma_N p^2 \qquad (N = 1, ..., 7). \tag{3}$$

The coefficients returned by the fit are given in Table 2.

We also did a fit over a wider potential temperature and salinity range shown in Table 3 in order to cover extreme temperatures and make the formula applicable in brackish water. The corresponding coefficients $\tilde{C}_{1...7}$ are given in Table 4.

The fit was performed using the software package *Mathematica* (Wolfram, 1991). We solved for the coefficients $C_{1...7}$ of (2) that minimize the integral of the squared difference between the exact and approximate functions. The integral is taken over the given range of θ and S, at a fixed value of p, called p_0 below:

$$\int_{S_1}^{S_2} \int_{\theta_1}^{\theta_2} [\sigma(\theta, S, p_0) - \rho(\theta, S, p_0)]^2 dS \, d\theta = \min. \tag{4}$$

To find the minimum in the space of the seven C_N's, we take the derivative with respect to each C_N and set the resulting expression to zero:

$$\nabla_{C_{1...7}} \int_{S_1}^{S_2} \int_{\theta_1}^{\theta_2} [\sigma(\theta, S, p_0) - \rho(\theta, S, p_0)]^2 dS \, d\theta = 0. \tag{5}$$

Since only $\sigma(\theta, S, p_0)$ depends on C_N, this can be written as:

$$\int_{S_1}^{S_2} \int_{\theta_1}^{\theta_2} 2[\sigma(\theta, S, p_0) - \rho(\theta, S, p_0)][\nabla_{C_{1...7}} \sigma(\theta, S, p_0)] dS \, d\theta = 0. \tag{6}$$

We use Mathematica to evaluate the integral numerically, and then solve the resulting set of linear equations for the coefficients C_N. After this is done for all 50 values of p, a quadratic is fitted to each set of (p, C_N) points to obtain the coefficients α_N, β_N, and γ_N.

	θ	S	p
	$-2°C \leq \theta \leq 30°C$	$30\% \leq S \leq 38\%$	$0 \leq p \leq 50\,\mathrm{MPa}$

Table 1: "Narrow" range of variables used for polynomial fit.

N	α_N	β_N	γ_N
1	-1.36471×10^{-1}	5.06423×10^{-1}	-5.52640×10^{-4}
2	4.68181×10^{-2}	-3.57109×10^{-3}	4.88584×10^{-6}
3	8.07004×10^{-1}	-8.76148×10^{-4}	9.96027×10^{-7}
4	-7.45353×10^{-3}	5.25243×10^{-5}	-7.25139×10^{-8}
5	-2.94418×10^{-3}	1.57976×10^{-5}	-3.98736×10^{-9}
6	3.43570×10^{-5}	-3.46686×10^{-7}	4.00631×10^{-10}
7	3.48658×10^{-5}	-1.68764×10^{-7}	8.26368×10^{-11}

Table 2: Coefficients of the approximation $C_N(p) = \alpha_N + \beta_N p + \gamma_N p^2$ [p in MPa] resulting from the two-stage least-squares fitting procedure over the θ, S, p range shown in Table 1.

$\tilde{\theta}$	$\tilde{S}$	$\tilde{p}$
$-2°C \leq \tilde{\theta} \leq 40°C$	$0\% \leq \tilde{S} \leq 42\%$	$0 \leq \tilde{p} \leq 100\,\mathrm{MPa}$

Table 3: A wider range of variables for polynomial fit.

N	$\tilde{\alpha}_N$	$\tilde{\beta}_N$	$\tilde{\gamma}_N$
1	-9.20601×10^{-2}	5.07043×10^{-1}	-5.43283×10^{-4}
2	5.10768×10^{-2}	-3.69119×10^{-3}	6.54837×10^{-6}
3	8.05999×10^{-1}	-9.34012×10^{-4}	1.38777×10^{-6}
4	-7.40849×10^{-3}	5.33243×10^{-5}	-1.01563×10^{-7}
5	-3.01036×10^{-3}	1.75145×10^{-5}	-2.34892×10^{-8}
6	3.32267×10^{-5}	-3.25887×10^{-7}	4.98612×10^{-10}
7	3.21931×10^{-5}	-1.65849×10^{-7}	2.17612×10^{-10}

Table 4: Same as Table 2, but based on the wide θ, S, p range shown in Table 3.

3 Results

To convey an impression of the accuracy of the fit, we show in Fig. 1 the density anomaly $\sigma = \rho$ - $1000 \, \mathrm{kg \, m^{-3}}$ as a function of θ and S at three pressure levels (0, 20, and $40 \, \mathrm{MPa}$, referred to as σ_0, σ_2, and σ_4 respectively), using Table 2 and Table 4 respectively. Since the isopycnals obtained from the JMcD formula (1) and from the approximation (2) are indistinguishable in these plots, we plot the difference between (2) and (1) as dashed lines. In Fig. 1(a), the difference is of order $10^{-3} \, \mathrm{kg \, m^{-3}}$, four orders of magnitude smaller than the density anomaly (σ) itself. The maximum error is 0.0065 $\mathrm{kg \, m^{-3}}$. A check value for density computed using (2) and Table 2 is $\sigma(\theta = 1^{\circ}C, S = 35, p = 50 \, \mathrm{MPa}) = 50.402762 \, \mathrm{kg \, m^{-3}}$. A much bigger difference is shown in Fig. 1(b) due to the wider fitting range.

The coefficients $C_{1...7}$ in (2) determined at various pressure levels using Table 2 are plotted in Fig. 2. Their almost linear variation with pressure indicates that a quadratic fit in p is sufficient in (3). The root-mean-square (rms) of the difference of (2) and (1), when using Table 2, lies between $2.67 \times 10^{-3} \, \mathrm{kg \, m^{-3}}$ at the surface and $1.85 \times 10^{-3} \, \mathrm{kg \, m^{-3}}$ at $50 \, \mathrm{MPa}$, which at most depths is smaller than the rms error shown in LI. Consistent with the results presented in Fig. 1, the rms error using Table 4 is much larger, since the latter formula is a fit over a much wider range of θ, S, p. Thus, while fairly reproducing the density of brackish and extremely warm/salty water, this formula sacrifices accuracy in the water masses that make up the bulk of the world ocean.

In summary, the coefficients given in Table 2 are recommended for use in global and basin-scale circulation modeling where infusions of fresh water and localized temperature extremes play only a minor role. Estuarine and/or marginal sea models may require use of the coefficients given in Table 4.

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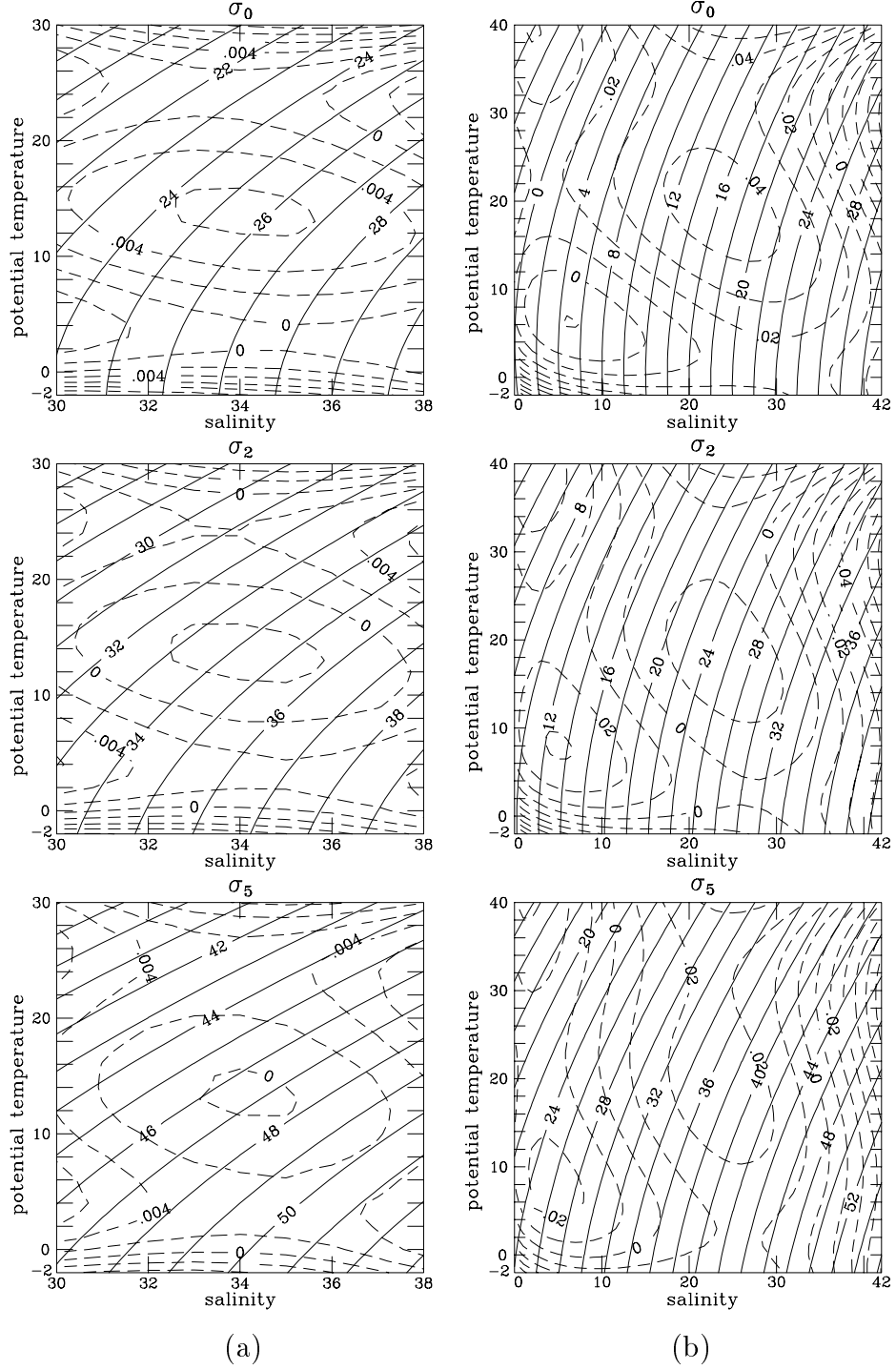Wolfram, S. *Mathematica,* 961 pp., Addison-Wesley, Redwood City, Calif., 1991.

Figure 1: σ_0, σ_2, and σ_5 $(\mathrm{kg\,m^{-3}})$ in θ-S diagram. (a) using Table 2; (b) using Table 4. Solid: JMcD formula (1); dashed: (2) minus JMcD formula.
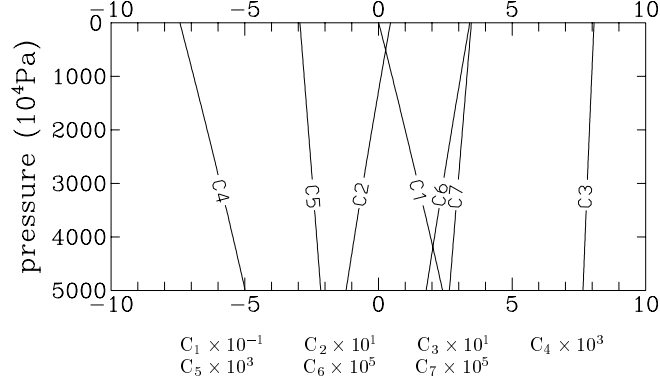
Figure 2: Coefficients in (2) as functions of pressure, based on narrow θ, S, p range in Table 1.
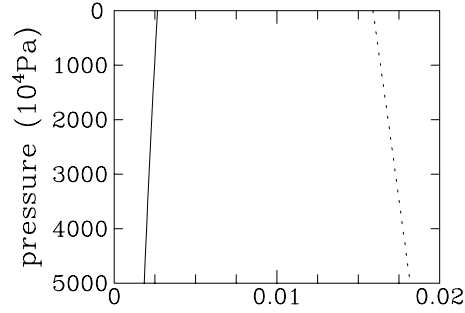

Figure 3: Rms error of (2) with respect to JMcD formula as function of pressure. Solid: coefficients in Table 2 evaluated in the narrow θ, S, p range shown in Table 1; dashed: coefficients in Table 4 evaluated in the wide θ, S, p range shown in Table 3.